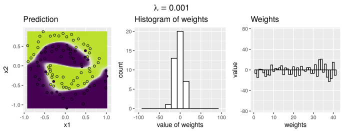
Introduction to Machine Learning

Regularization
Non-Linear Models and Structural Risk Minimization



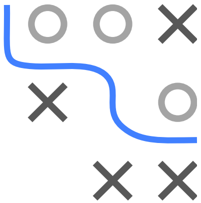
Learning goals

- Understand that regularization and parameter shrinkage can be applied to non-linear models
- Know structural risk minimization

SUMMARY: REGULARIZED RISK MINIMIZATION

If we should define (supervised) ML in only one line, this might be it:

$$\min_{\boldsymbol{\theta}} \mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \min_{\boldsymbol{\theta}} \left(\sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right) + \lambda \cdot J(\boldsymbol{\theta}) \right)$$

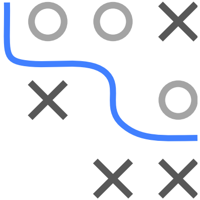


We can choose for a task at hand:

- the **hypothesis space** of f, which determines how features can influence the predicted y
- the **loss** function L, which measures how errors should be treated
- the **regularization** $J(\boldsymbol{\theta})$, which encodes our inductive bias and preference for certain simpler models

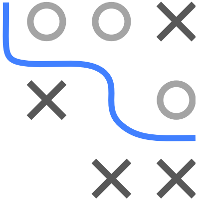
By varying these choices one can construct a huge number of different ML models. Many ML models follow this construction principle or can be interpreted through the lens of regularized risk minimization.

REGULARIZATION IN NONLINEAR MODELS

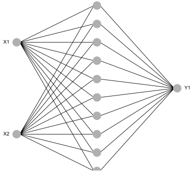


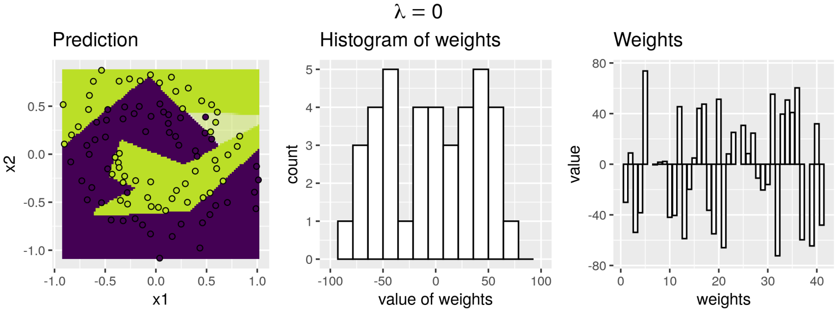
- So far we have mainly considered regularization in LMs.
- Can also be applied to non-linear models (with numeric parameters), where it is often important to prevent overfitting.
- Often, non-linear models can be seen as LMs based on internally transformed features.
- Here, we typically use $L2$ regularization, which still results in parameter shrinkage and weight decay.
- Adding regularization is commonplace and sometimes crucial in non-linear methods such as NNs, SVMs, or boosting.
- By adding regularization, prediction surfaces in regression and classification become smoother.

REGULARIZATION IN NONLINEAR MODELS



Classification for the `spirals` data. Neural network with single hidden layer containing 10 neurons, regularized with $L2$:





Varying λ affects smoothness of the decision boundary and magnitude of network weights

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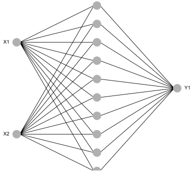

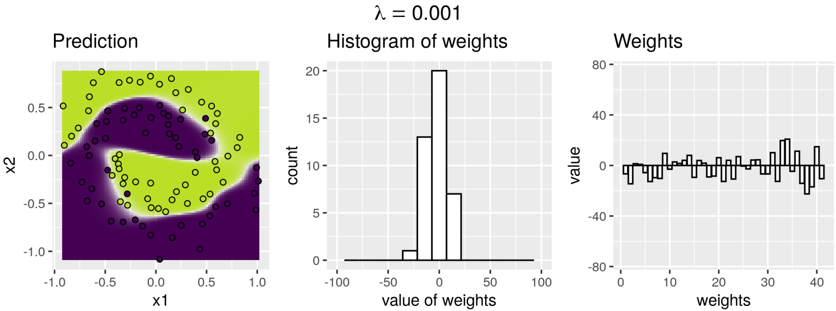

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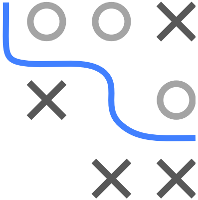

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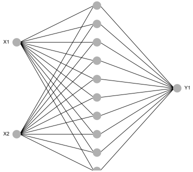

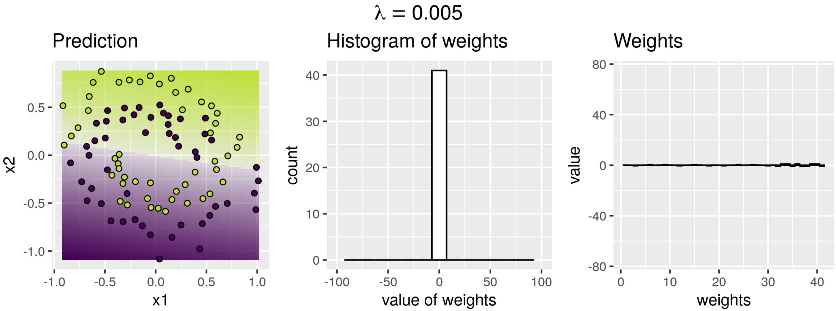

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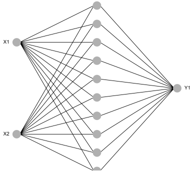

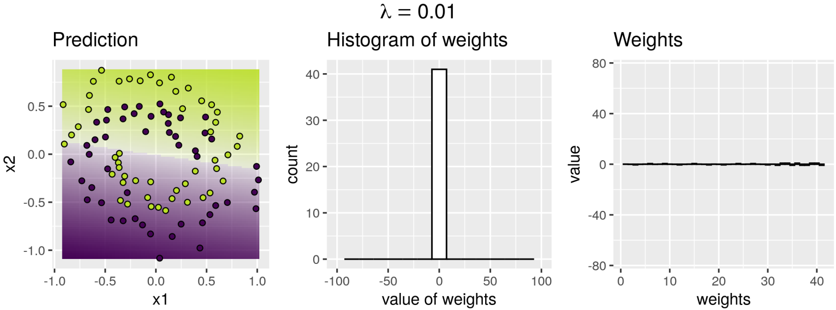

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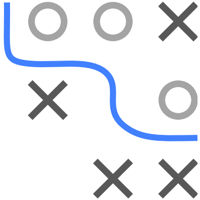
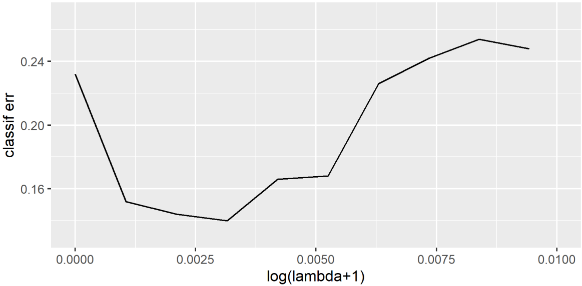
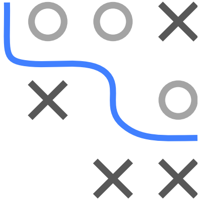


The prevention of overfitting can also be seen in CV. Same settings as before, but each λ is evaluated with repeated CV (10 folds, 5 reps).

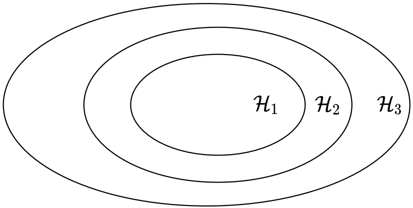


We see the typical U-shape with the sweet spot between overfitting (LHS, low λ) and underfitting (RHS, high λ) in the middle.

STRUCTURAL RISK MINIMIZATION

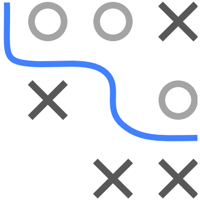


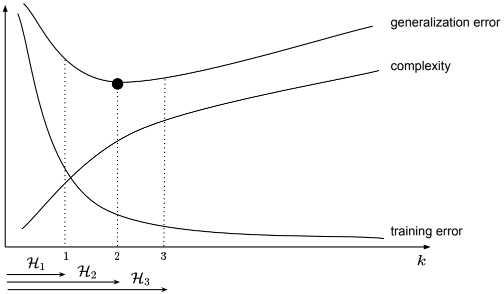
- Thus far, we only considered adding a complexity penalty to empirical risk minimization.
- Instead, structural risk minimization (SRM) assumes that the hypothesis space $\mathcal{H}$ can be decomposed into increasingly complex hypotheses (size or capacity): $\mathcal{H} = \cup_{k \geq 1} \mathcal{H}_k$.
- Complexity parameters can be, e.g. the degree of polynomials in linear models or the size of hidden layers in neural networks.



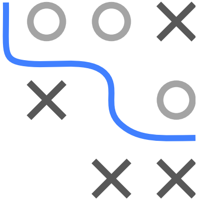
STRUCTURAL RISK MINIMIZATION / 2

- SRM chooses the smallest k such that the optimal model from $\mathcal{H}_k$ found by ERM or RRM cannot significantly be outperformed by a model from a $\mathcal{H}_m$ with $m > k$.
- By this, the simplest model can be chosen, which minimizes the generalization bound.
- One challenge might be choosing an adequate complexity measure, as for some models, multiple complexity measures exist.



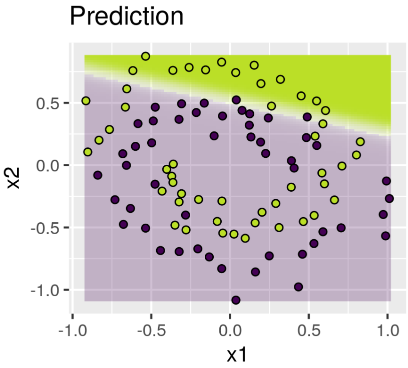


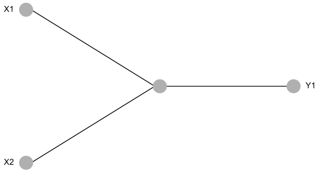
STRUCTURAL RISK MINIMIZATION



Classification for the `spirals` data. NN with 1 hidden layer, and fixed (small) L2 penalty.
Varying the size of the hidden layer affects smoothness of the decision boundary:

size of hidden layer = 1



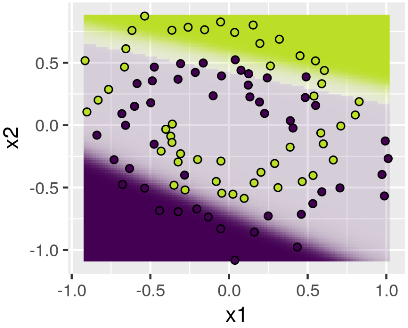


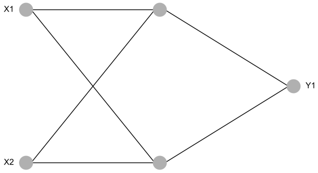
STRUCTURAL RISK MINIMIZATION

Classification for the `spirals` data. NN with 1 hidden layer, and fixed (small) L2 penalty.
Varying the size of the hidden layer affects smoothness of the decision boundary:

size of hidden layer = 2

Prediction



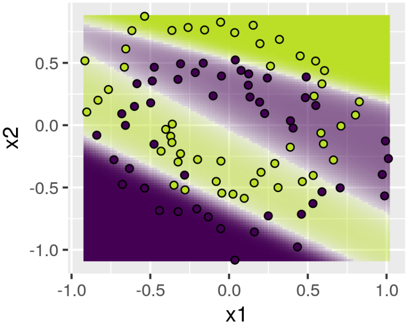


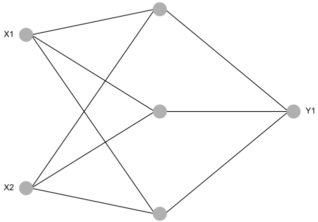
STRUCTURAL RISK MINIMIZATION

Classification for the `spirals` data. NN with 1 hidden layer, and fixed (small) L2 penalty.
Varying the size of the hidden layer affects smoothness of the decision boundary:

size of hidden layer = 3

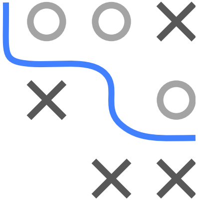
Prediction



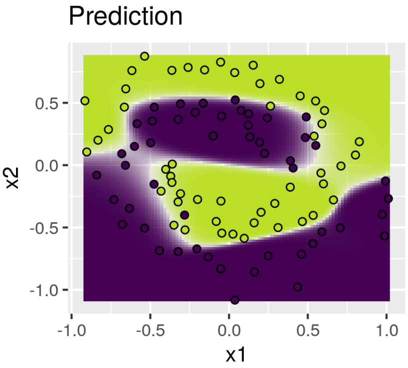


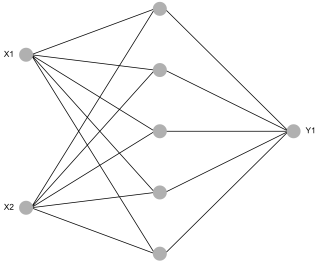
STRUCTURAL RISK MINIMIZATION

Classification for the `spirals` data. NN with 1 hidden layer, and fixed (small) L2 penalty.
Varying the size of the hidden layer affects smoothness of the decision boundary:



size of hidden layer = 5

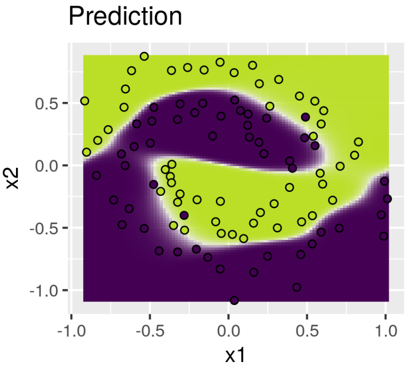


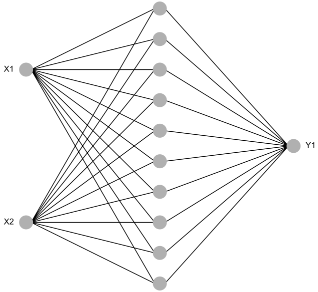


STRUCTURAL RISK MINIMIZATION

Classification for the `spirals` data. NN with 1 hidden layer, and fixed (small) L2 penalty.
Varying the size of the hidden layer affects smoothness of the decision boundary:

size of hidden layer = 10

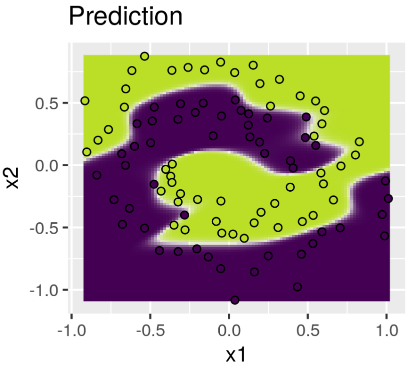


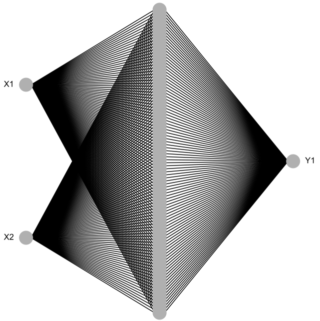


STRUCTURAL RISK MINIMIZATION

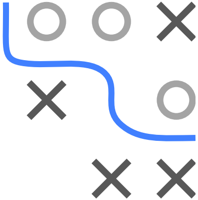
Classification for the `spirals` data. NN with 1 hidden layer, and fixed (small) L2 penalty.
Varying the size of the hidden layer affects smoothness of the decision boundary:

size of hidden layer = 100

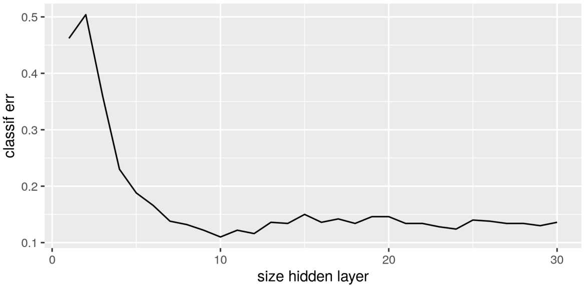




STRUCTURAL RISK MINIMIZATION

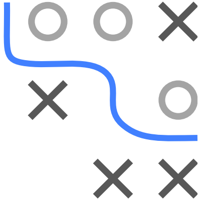


Again, complexity vs CV score.



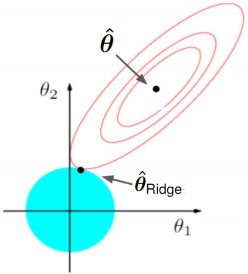
A minimal model with good generalization seems to have ca. 10 hidden neurons.

STRUCTURAL RISK MINIMIZATION AND RRM



Note that normal RRM can also be interpreted through SRM, if we rewrite the penalized ERM as constrained ERM.

$$
\begin{aligned}
\min_{\boldsymbol{\theta}} \quad & \sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right) \\
\text{s.t.} \quad & \|\boldsymbol{\theta}\|_2^2 \leq t
\end{aligned}
$$



We can interpret going through λ from large to small as through t from small to large. This constructs a series of ERM problems with hypothesis spaces $\mathcal{H}_\lambda$, where we constrain the norm of $\boldsymbol{\theta}$ to unit balls of growing size.